

Spectral Report for Qualitative Unknown Lab

Unknown Number _____

1. **Infrared Spectrum** - On your IR spectrum, label ALL peaks of importance for corresponding bond vibration and indicate what bond is associated with what peak.
2. **Elemental Analysis**: Show calculations for obtaining the empirical formula

%C _____ %H _____ %O _____ %X _____

Empirical Formula: _____

Calculate the molecular weight based on the empirical formula:

3. **Mass spectrum**. Identify the following pertinent peaks:

Presence of halide? Yes No MS Peak(s) _____

Presence of alcohol Yes No MS Peak(s) _____

Molecular ion _____

Base peak _____

Does the molecular ion match the molecular weight of the empirical formula? _____

If no, what is the ratio between the molecular ion and the molecular weight of the empirical formula?

Write the molecular formula, based on this information: _____

Proton NMR:

Integration ratio (show calculations): _____

Now draw the fragments that you can determine from your Proton NMR:

Chemical Shift

Split Pattern

Integration

Molecular Fragment

Final Result:

1. Structure of Unknown Compound:

2. Supporting information for how you reached your conclusion:

If your compound is aromatic, identify how you know its mono or disubstituted.

If your compound is aromatic and disubstituted, identify how you know its ortho, meta or para.

If your compound has a halide, explain how you know which halide it is.